

# NATIONAL BUREAU OF STANDARDS REPORT

8521

PRELIMINARY REPORT ON A SURVEY OF  
THERMODYNAMIC PROPERTIES OF THE COMPOUNDS OF THE ELEMENTS CHNOPS

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to

National Aeronautics and Space Administration

1 August 1964

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U. S. DEPARTMENT OF COMMERCE  
NATIONAL BUREAU OF STANDARDS

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\* NBS Group, Joint Institute for Laboratory Astrophysics at the University of Colorado.

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# NATIONAL BUREAU OF STANDARDS REPORT

## NBS PROJECT

221-11-0429

1 August 1964

## NBS REPORT

8521

### A SURVEY OF THERMODYNAMIC PROPERTIES OF THE COMPOUNDS OF THE ELEMENTS CHNOPS

George T. Armstrong, George T. Furukawa, and  
Joseph Hilsenrath

Heat Division

Progress Report for the Period Ending 31 July 1964

to

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

Contract No. R-138

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U. S. DEPARTMENT OF COMMERCE  
NATIONAL BUREAU OF STANDARDS

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## FOREWORD

A study at the National Bureau of Standards (NBS), of which this is the first progress report, has been undertaken to meet the need of the National Aeronautics and Space Administration (NASA) for thermodynamic information on biologically related materials important to the space program for several reasons. Among these reasons are the necessity of inferring the maximum amount of useful chemistry of incompletely accessible environments, for which only limited information is available; the possibility of the occurrence of organic compounds naturally synthesized under primitive conditions, and the possibility of theoretically recovering part of the prebiological history of the earth.

This program is being carried out under the technical supervision of Dr. George Jacobs of NASA, and with the consultation of Dr. Harold Morowitz of the Yale University, Department of Molecular Biology and Biophysics, and Dr. C. W. Beckett of the Heat Division (NBS). The contract (Contract No. R-138) was initiated May 1, 1964, and this report covers the first three months of the term of the contract.

*George T. Armstrong*

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George T. Armstrong  
Supervisory Chemist  
Project Leader

## Section I

### SUMMARY OF PROGRESS ON THE SURVEY OF THERMODYNAMIC DATA

The survey of literature and available thermodynamic data falls naturally into two categories which are carried out by different personnel and are separately described in this Report. The two categories are (1) heat capacities, enthalpies and entropies, carried out under the supervision of G. T. Furukawa, and (2) heats and free energies of reaction and formation, under the supervision of G. T. Armstrong. These surveys are discussed briefly in parts A and B respectively, of Section I, and the summarized or illustrative findings are given in Section II and Section III respectively. The findings listed in Sections II and III are not necessarily in a final form, but the formats presented are shown, at least in part to test their utility.

#### Part A. Heat Capacity of Compounds of Hydrogen, Carbon, Nitrogen, Oxygen, Phosphorus, and Sulfur

by

George T. Furukawa

The literature survey of heat-capacity data was initiated as a part of the program to investigate the thermodynamic properties of biologically related compounds of the elements: H, C, N, O, P and S. The heat-capacity data will be analyzed to obtain tables of thermodynamic properties.

Section II of this report gives the results of the literature survey of heat capacity of compounds containing H, C, N, O, and S. The survey on phosphorus compounds will be started during the next quarter. The literature survey is still in progress and other sources of data and data on other compounds are being compiled. The data on most of the important compounds are considered, however, to have now been compiled. The slower, more time consuming process of data analysis is in progress to obtain tables of thermodynamic properties.

The substances on which heat-capacity data are available, were subdivided temporarily into the following classifications until more convenient ones could be devised:

1. alcohols, aliphatic
2. alcohols, aromatic
3. alcohols, polyhydroxy, aliphatic
4. sugars
5. ketones
6. esters
7. ethers
8. aldehydes
9. acids, aliphatic
10. acids, aromatic

11. acids, hydroxy, mercapto, and polycarboxylic
12. amines and other C-N compounds
13. sulfur compounds, thiol group
14. sulfur compounds, thia, dithia, and cyclic groups
15. amino acids, aliphatic groups
16. amino acids, hydroxyl containing, aliphatic and aromatic groups
17. amino acids, aromatic and related groups
18. amino acids, carboxyl and amide groups
19. amino acids, amino groups
20. amino acids, sulfur containing groups
21. amino acids, imino acid groups
22. other biologically important compounds:  
peptide bond
23. other biologically important compounds:  
guanido group
24. other biologically important compounds:  
purines and others

The sources of the existing data are arranged tabularly along with the temperature range over which the heat capacity or relative enthalpy measurements were obtained. The physical states of the substances in the above range of measurements are indicated by the symbols c, l, g, or gl, which designate the crystal, liquid, gaseous, or glassy state, respectively. The entropy at 298.15°K or at another temperature is given whenever it was evaluated by the investigator from the data. The temperature corresponding to the entropy value is given whenever the temperature is other than 298.15°K. The physical state corresponding to the value of entropy is given in the parenthesis wither preceding or following the value. The entropy value is enclosed in parenthesis whenever the value was estimated or obtained by extrapolation. The numbers in brackets are the literature references listed at the end of this chapter. The unit of calorie is the defined calorie = 4.1840 Joules.

Part B. Survey of Data on Heats of Reaction and Formation  
by G. T. Armstrong

Pending the establishment of more definite limits on the scope of compounds to be covered ultimately in the survey, the literature compilation was started with a group of amino acids, on the bases that (1) this class of substances must definitely be of interest, (2) they are a sufficiently clearly characterized group of compounds so that the data on them should be readily found, and (3) we were aware of set of measurements of heats of formation on a series of a few of them, which might well be definitive for them. The search so far completed covers amino acids and a very few related compounds encountered in the search for them. The information so far compiled comprises some 50 odd compound-studies. (Some sources discuss more than one compound; some compounds were studied more than once.) The findings are summarized in Section III of this report.

The compound studies have been listed in a logical alphabetic-numeric order with respect to the elemental composition of the compound. The order thus far adopted, and which we propose to use for the remainder of the work is almost precisely that in which the same compounds would be found in the Chemical Abstracts Formula Index. The only exception is in the treatment of water of hydration of crystals. In our classification this will be compiled directly into the elemental composition of the compound, and the resulting formula will be classified according to the composition thus shown. The alphabetical order in principle differs somewhat from the order in Chemical Abstracts Index for organic compounds, for which they invariably follow C by H regardless of other elements. However, in the special case formed by the six elements C-H-N-O-P-S, no elements intervene alphabetically between C and H, and so no deviation from the Chemical Abstracts Index occurs. The order of the compounds is of some importance because their number will run into the hundreds, and it is necessary to make finding practicable.

Some attention was given to the manner of presenting information. A card file has been established, in which there is a separate card for each compound-study. So far listed on these cards are: elemental composition, systematic name, linear structural formula, trivial or common name, class of substance, source reference, and source-reference finding number. This information has been placed on punched tape, and so the information can be reproduced readily by automatic typewriter at will. Some additional information will be added ultimately, such as the heat or equilibrium process observed, and the quantity reported for that process. The finding numbers for the sources in this study have the prefix BIO - for biological, to distinguish them from our other records.

The material in Section III is that shown on the cards, as reproduced by means of the tapes. It is illustrated here in an experimental way, to begin to evaluate the utility of this manner of storage and presentation. Changes may be incorporated in the system when they are seen to be desirable.

Some general sources of information are known for organic compounds which are of sufficient interest to be mentioned here.

- (1) A review by K. Burton "Free Energy Data of Interest in Biochemistry" lists approximately 100 substances and is found as an appendix in the booklet:  
Energy Transformation in Living Matter, a Survey, by H. A. Krebs and H. L. Kornberg, (Springer Verlag, Berlin, 1957). This booklet is available separately but is reprinted from Ergebniss der Physiologie, Biologischen Chemie und Experimentellen Pharmacologie 49, 213-298 (1957).
- (2) Heats of Combustion of Organic Compounds, by M. S. Kharasch, Bureau of Standards J. Research 2, 359-430 (1929). This was the most extensive compilation at the time of its appearance, and while now too old to be nearly complete, it does list practically all of the early literature. Perhaps 1000 compounds are listed.
- (3) Chemistry of the Amino Acids. Volume I. J. P. Greenstein and M. Winitz, (Wiley and Sons, New York, 1961). Chapter 5, Thermodynamics and Solubility gives a review of thermodynamic data on the amino acids.

Primarily, in order to provide guidance in the survey of thermochemical data, a planning session was held August 6, 1964. While this date is after the close of this reporting period, the meeting was held before the typewriting of this report was completed, and so a memorandum pertaining to it is attached as an appendix to this report.

Section II

PRELIMINARY COMPILATION OF HEAT CAPACITY AND RELATIVE ENTHALPY  
AND ENTROPY DATA PUBLISHED ON BIOLOGICALLY RELATED SUBSTANCES

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy 298.15°K cal/deg-mole	7 Ref.
<b>1. Alcohols, aliphatic</b>						
Methyl alcohol, $\text{CH}_3\text{OH}$	c, l	1925	89-290		32.6 (l)	[38]
	c, l	1925	89-290			[4]
	c, l	1929	19-292		30.3 ± 0.2 (l)	[1]
	l	1929	190-265			[24]
	c	1937	4-28		30.3 (l)	[15]
ethyl alcohol, $\text{CH}_3\text{CH}_2\text{OH}$	l	1908	182-245			[25]
	c	1920	88-141			[58]
	l	1920	196-271			[58]
	c, l	1925	87-298		42.3 (l)	[38]
	c, l	1929	19-294		38.4 ± 0.3 (l)	[2]
	l	1929	184-269			[24]
	gl	1920	86-96			[58]
	gl	1925	87-110			[38]
	gl, l	1927	87-298			[11]
	gl, l	1929	18-108			[2]
	1929	$S^\circ(l, 298) - S^\circ(gl, 0) = 35.8$				[2]
	1929	$S^\circ(gl, 0) = 2.6$				[2]
n-propyl alcohol, $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$	c, l	1926	88-275		51.2 (l)	[6]
	l	1929	163-274			[24]
	gl	1913	20-80			[31]
	gl, l	1920	77-275			[58]
	gl, l	1926	86-275			[6]
	gl, l	1927	86-275			[11]
ethyl alcohol-n-propyl alcohol, $\text{CH}_3\text{CH}_2\text{OH}-n\text{-CH}_3\text{CH}_2\text{CH}_2\text{OH}$ , equimolar mixture	gl, l	1920	78-273			[58]

Section II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy 298.15°K cal/deg-mole	7 Ref.
isopropyl alcohol, $\text{CH}_3\text{CHOHCH}_3$	c, l	1925	71-293		45.6 (l)	[37]
	c, l	1928	71-293		46.1 (l)	[12]
	c, l	1929	19-293		43.0 ± 0.3 (l)	[3]
n-butyl alcohol, $\text{CH}_3(\text{CH}_2)_2\text{CH}_2\text{OH}$	c, l	1925	91-294		60.2 (l)	[38]
sec.-butyl alcohol, $\text{CH}_3\text{CHOHCH}_2\text{CH}_3$	gl, l	1936	103-282			[14]
tert.-butyl alcohol, $(\text{CH}_3)_3\text{COH}$	c, l	1903		251-318		[17]
	c, l	1926	87-300		47.2 (l)	[5]
n-amyl alcohol, $\text{CH}_3(\text{CH}_2)_3\text{CH}_2\text{OH}$	c, l	1933	94-298		60.9 (l)	[61]
tert.-amyl alcohol, $(\text{CH}_3)_2\text{COH-CH}_2\text{CH}_3$	c, l	1933	92-294		54.8 (l)	[61]
cyclopentanol, $(\text{CH}_2)_4\text{CHOH}$	c, l	1959	80-300		49.3 (l)	[26]
furfuryl alcohol, $\text{C}_4\text{H}_3\text{OCH}_2\text{OH}$	c, l	1959	90-300		51.6 (l)	[26]
n-hexyl alcohol, $\text{CH}_3(\text{CH}_2)_4\text{CH}_2\text{OH}$	c, l	1929	18-290		68.6 ± 0.4 (l)	[2]
n-heptyl alcohol, $\text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{OH}$	c, l	1959	80-300		77.9 (l)	[26]
cetyl alcohol, $\text{CH}_3(\text{CH}_2)_{14}\text{CH}_2\text{OH}$	c	1959	80-290		108.0 (c)	[26]

Section II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy 298.15°K cal/deg-mole	7 Ref.
<b>2. Alcohols, aromatic</b>						
phenol, $C_6H_5OH$	c	1925		89-290		[4]
	c	1933	93-296		34.1 (c)	[61]
	c	1935	78-229			[23]
benzyl alcohol, $C_6H_5CH_2OH$	c, l	1936	90-300		51.8 (l)	[8]
hydroquinone, $p-C_6H_4(OH)_2$	c	1924	28-274			[19]
pyrocatechol, $o-C_6H_4(OH)_2$	c, l	1926		293-473		[75]
resorcinol, $m-C_6H_4(OH)_2$	c, l	1926		293-473		[75]
$\alpha$ -naphthol, $C_{10}H_7OH$	c, l	1926		293-453		[75]
$\beta$ -naphthol, $C_{10}H_7OH$	c, l	1926		293-478		[75]
<b>3. Alcohols, polyhydroxy, aliphatic</b>						
ethylene glycol $(CH_2OH)_2$	c, l	1901		250-412		[16]
	c, l	1925	88-293		42.9 (l)	[37]
propylene glycol, $CH_3CHOHCH_2OH$	gl, l	1927	91-277			[11]

Section II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy 298.15°K cal/deg-mole	7 Ref.
glycerol, $(\text{CH}_2\text{OH})_2\text{CHOH}$	c l c gl, l gl, l gl gl, l gl gl	1923 1925 1937 1922 1923 1926 1927 1937 1937	70-280 3-87 19-294 70-299 11-13 70-299 2-95 167-193		53.2 (l) 48.87 (l)	[59] [37] [15] [40] [59] [39] [11] [15] [69]
erythritol, $(\text{CH}_2\text{OHCHOH})_2$	c	1926	87-292		42.5 (c)	[5]
$\alpha$ -monopalmitin, $\text{CH}_2\text{OHCHONCH}_2\text{OCO}(\text{CH}_2)_{14}\text{CH}_3$	c	1940	298			[65]
$\beta$ -monopalmitin, $(\text{CH}_2\text{OH})_2\text{CHOCO}(\text{CH}_2)_{14}\text{CH}_3$	c	1940	298			[65]
dulcitol, $\text{CH}_2\text{OH}(\text{CHOH})_4\text{CH}_2\text{OH}$	c	1926	88-293		59.2 (c)	[6]
d-mannitol, $\text{CH}_2\text{OH}(\text{CHOH})_4\text{CH}_2\text{OH}$	c	1926	88-294		60.5 (c)	[5]
<u>4. Sugars</u>						
glucose, $\text{C}_6\text{H}_{12}\text{O}_6$	c c c gl, l gl	1922 1925 1951 1928 1941	20-296 273-368 94-340 273-333	53.4 (c)		[40] [37] [48] [13] [68]

## SECTION II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy 298.15°K cal/deg-mole	7 Ref.
<i>L</i> -sorbose, $C_6H_{12}O_6$	c	1941	64-296		52.8 (c)	[67]
$\alpha$ -D-galactose, $C_6H_{12}O_6$	c	1941	64-297		49.1 (c)	[67]
$\alpha$ -lactose monohydrate, $C_{12}H_{22}O_{11}\cdot H_2O$	c	1941	61-297		99.1 (c)	[66]
$\beta$ -lactose, $C_{12}H_{22}O_{11}$	c c	1936 1941	83-298 66-289		96.4 (c) 92.3 (c)	[64] [66]
$\beta$ -maltose monohydrate, $C_{12}H_{22}O_{11}\cdot H_2O$	c	1941	61-296		99.8 (c)	[66]
sucrose, $C_{12}H_{22}O_{11}$	c c	1933 1950	94-297 276-300		86.1 (c)	[61] [63]
<b>5. Ketones</b>						
acetone, $(CH_3)_2CO$	c, l c, l c, l c, l l	1925 1925 1928 1929 1929	70-289 89-290 70-289 18-297 205-256		52.0 (l) 52.7 (l) 47.9 ± 0.3 (l)	[37] [4] [12] [3] [24]
methyl ethyl ketone, $CH_3COCH_2CH_3$	c, l	1959	80-300		57.7 (l)	[26]
benzophenone, $(C_6H_5)_2CO$	c, l gl, l	1910 1910		80-314 80-314		[21] [21]
quinone, $C_6H_4O_2$	c c, l	1924 1926	22-291 293-433			[19] [75]
quinhydrone, $C_6H_4O_2\cdot C_6H_4(OH)_2$	c	1924	20-243			[19]

Section II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy 298.15°K cal/deg-mole	7 Ref.
6. <u>Esters</u>						
ethyl acetate, $\text{CH}_3\text{CH}_2\text{OCOCH}_3$	c, l	1933	92-294		62.0 (l)	[61]
$\beta$ -naphthyl salicylate, $\text{HOC}_6\text{H}_4\text{COOC}_{10}\text{H}_7$	c, l gl, l	1910 1910		83-350 82-362		[21] [21]
7. <u>Ethers</u>						
dimethyl ether, $(\text{CH}_3)_2\text{O}$	c, l	1941	14-245		$(44.98 \pm 0.40)(l)$ $(63.72 \pm 0.20)(g)$	[76] [76]
				$S^\circ(l, 200.00) = 35.03 \pm 0.07$ $S^\circ(g, 200.00) = 58.03 \pm 0.10$		[76] [76]
diethyl ether, $(\text{CH}_3\text{CH}_2)_2\text{O}$	c, l c, l	1926 1935	76-290 80-255		67.7	[6] [23]
dL-isopropyl ether, $[(\text{CH}_3)_2\text{CH}]_2\text{O}$	c, l	1933	92-293		70.4 (l)	[61]
ethylene oxide, $(\text{CH}_2)_2\text{O}$	c, l	1949	15-284			[70]
				$S^\circ(l, 283.60) = 35.72$ $S^\circ(g, 283.60) = 57.38$		[70] [70]
furan, $\text{C}_4\text{H}_4\text{O}$	c, l	1952	12-300		$42.22 \pm 0.08(l)$ $63.86 \pm 0.10(g)$	[99] [99]
1,4-dioxane, $(\text{OCH}_2\text{CH}_2)_2$	c, l	1934	93-298		47.0 (l)	[103]
8. <u>Aldehydes</u>						
n-butyaldehyde, $\text{CH}_3(\text{CH}_2)_2\text{CHO}$	c, l	1959	80-300		59.0 (l)	[26]
n-heptaldehyde, $\text{CH}_3(\text{CH}_2)_5\text{CHO}$	c, l	1959	80-300		83.3 (l)	[26]

Section II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy 298.15°K cal/deg-mole	7 Ref.
<b>9. Acids, aliphatic</b>						
formic acid, HCOOH	c, l c, l	1920 1941	71-292 15-300		34.2 (l) 30.82 ± 0.1 (l)	[57] [62]
acetic acid, $\text{CH}_3\text{COOH}$	c c, l	1913 1925	20-80 87-275		46.3 (l)	[31] [37]
propanoic acid, $\text{CH}_3\text{CH}_2\text{COOH}$	c	1909	227-253			[18]
n-butyric acid, $\text{CH}_3(\text{CH}_2)_2\text{COOH}$	c, l	1926	89-291		61.0 (l)	[5]
palmitic acid, $\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$	c	1925	88-292		129.9 (c)	[37]
<b>10. Acids, aromatic</b>						
benzoic acid, $\text{C}_6\text{H}_5\text{COOH}$	c, l c c, l c c c, l c	1926 1933 1951 1956 1957 1960 1960	293-473 93-295 14-410 80-298 20-294 4-407 11-303	293-473 40.8 (c) 40.05 (c) 40.11 (c) 40.04 (c)		[75] [61] [73] [74] [71] [72] [47]
ortho-toluic acid, $\text{CH}_3\text{C}_6\text{H}_4\text{COOH}$	c, l	1926		293-473		[75]
meta-toluic acid, $\text{CH}_3\text{C}_6\text{H}_4\text{COOH}$	c, l	1926		293-443		[75]
para-toluic acid, $\text{CH}_3\text{C}_6\text{H}_4\text{COOH}$	c, l	1926		293-498		[75]

Section II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy cal/deg-mole	7 Ref.
ortho—aminobenzoic acid, $\text{NH}_2\text{C}_6\text{H}_4\text{COOH}$	c, l	1926		293-433		[75]
meta—aminobenzoic acid, c, l		1926		293-453		[75]
para—aminobenzoic acid, c, l		1926		293-463		[75]
11. <u>Acids, hydroxy, mercapto, and polycarboxylic</u>						
dl—lactic acid, $\text{CH}_3\text{CHOHCOOH}$	c, l gl, l	1936 1936	(90-300)* 96-303			[14] [14]
l(d)—lactic acid, $\text{CH}_3\text{CHOHCOOH}$	c	1940	84-298		34.00 (c)	[52]
d(l+)—lactic acid, $\text{CH}_3\text{CHOHCOOH}$	c	1940	84-293		34.30 (c)	[52]
$\beta$ -thiolactic acid, $\text{CH}_3\text{CHSHCOOH}$	c, l	1935	85-310		54.7 (l)	[7]
oxalic acid, $(\text{COOH})_2$	c c c c	1910 1910 1911 1925		84-273 84-202 84-202		[21] [22] [36] [37]
oxalic acid dihydrate, $(\text{COOH})_2 \cdot 2\text{H}_2\text{O}$	c c c	1910 1910 1911		82-273 84-198 84-198		[21] [22] [36]
succinic acid, $(\text{CH}_2\text{COOH})_2$	c	1930	93-290		42.0 (c)	[60]
fumaric acid, $(=\text{CHCOOH})_2$ , trans	c	1930	91-297		39.7 (c)	[60]

\*Estimated from data on glass and partially crystalline m.

Section II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy 298.15° cal/deg-mole	7 Ref.
maleic acid, $(=CHCOOH)_2$ , cis	c	1930	91-294		38.1 (c)	[60]
<i>l</i> -malic acid, $HOOCCH(OH)CH_2COOH$	c	1931			49. (c)	[56]
$\beta, \beta'$ -dithiodilactic acid, $(CH_2CHSHCOOH)_2$	c	1936	85-305		65.5 (c)	[7]
d-tartaric acid, $(CHOHCOOH)_2$	c	1906		83-287		[30]
	c	1914		83-328		[29]
o-phthalic acid, $O-C_6H_4(COOH)_2$	c	1936	90-300		49.7 (c)	[8]
phthalic anhydride, $C_6H_4(CO)_2O$	c	1936	90-300		42.7 (c)	[8]
12. <u>Amines and other C-N compounds</u>						
methylamine, $CH_3NH_2$	c, l	1937	13-259		(35.90) (l)	[35]
	l	1939	185-260	$S^\circ(l, 266.84) = 33.21$		[35]
						[34]
dimethylamine, $(CH_3)_2NH$	c, l	1939	14-280		$(43.58 \pm 0.05) (l)$	[32]
				$S^\circ(l, 280.04) = 41.55$		[32]
trimethylamine, $(CH_3)_3N$	c, l	1944	12-276		(49.82) (l)	[33]
				$S^\circ(l, 276.03) = 47.28 \pm 0.14$		[33]
aniline, $C_6H_5NH_2$	c, l	1933	94-298		45.8 (l)	[61]
urea, $(NH_2)_2CO$	c	1920	86-300		$41.0 \pm 2$ (c)	[57]
	c	1933	93-298		25.2 (c)	[61]
	c	1946	19-318		$25.00 \pm 0.05$ (c)	[49]
pyrrolidine, $(CH_2)_4NH$	c, l	1959	13-351		48.76 (l)	[84]
pyridine, $C_5H_5N$	c, l	1936	90-300		42.8 (l)	[8]
	c, l	1957	13-347		42.52 (l)	[87]

Section II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy 298.15° cal/deg-mole	7 Ref.
quinoline, $C_9H_7N$	c, l	1936	90-300		51.9 (l)	[ 8 ]
hydroxyacetanilide, $O, m, p - HOCH_3C_6H_4NHCOCH_3$	c, l	1926		323-413		[ 75 ]
cyanogen, $(CN)_2$	g c, l g	1936 1939 1939	173-279 15-252 185-320	$S^\circ(l, 251.95) = 33.19$ $(57.64) (g)$	[ 20 ] [ 27 ] [ 27 ] [ 28 ]	

13. Sulfur compounds, thiol group

methanethiol, $CH_3SH$	c, l	1942	15-271	$S^\circ(l, 279.12) = 39.01$ $S^\circ(g, 279.12) = 60.16 \pm 0.10$	[ 9 ]
ethanethiol, $CH_3CH_2SH$	c, l	1952	14-315	$49.48 \pm 0.10 (l)$ $70.77 \pm 0.15 (g)$	[ 96 ]
1-propanethiol, $CH_3(CH_2)SH$	c, l	1956	13-315	57.96 (l)	[ 79 ]
2-propanethiol, $CH_3CHSHCH_3$	c, l	1954	13-322	55.82 (l)	[ 81 ]
1-butanethiol, $CH_3(CH_2)_3SH$	c, l	1957	13-314	65.96 (l)	[ 86 ]
2-butanethiol, $CH_3CHSHCH_2CH_3$	c, l	1958	12-307	$64.87 (l)$ $87.67 (g)$	[ 88 ]
2-methyl-1-propanethiol, $CH_3CH(CH_3)CH_2SH$	c, l	1958	12-349	63.66 (l)	[ 85 ]
2-methyl-2-propanethiol, $(CH_3)_3CSH$	c, l	1953	12-329	$58.90 \pm 0.15 (l)$ $80.79 (g)$	[ 92 ]

## SECTION II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Enthalpy 298.15°K cal/deg-mole	7 Ref.
1-pentanethiol, $\text{CH}_3(\text{CH}_2)_4\text{SH}$	c, l	1952	13-321		$74.18 \pm 0.15 (\ell) [97]$ $99.18 \pm 0.35 (g) [97]$	
cyclopentanethiol, $\text{C}_5\text{H}_9\text{SH}$	c, l	1961	12-366		61.39 (l)	[90]
benzenethiol, $\text{C}_6\text{H}_5\text{SH}$	c, l c, l	1936 1958	90-300 13-375		52.6 (l) 53.25 (l)	[8] [78]

14. Sulfur compounds, thia, dithia and cyclic groups

thiapropane, $(\text{CH}_3)_2\text{S}$	c, l	1942	14-287	$(46.94 \pm 0.07) (\ell) [10]$ $(68.28 \pm 0.10) (g) [10]$		
				$S^\circ(\ell, 291.06) = 46.26$ $S^\circ(g, 291.06) = 67.87 \pm 0.1$	[10]	[10]
2-thiabutane, $\text{CH}_3\text{SC}_2\text{H}_5$	c, l	1951	14-298		$57.14 \pm 0.10 (\ell) [98]$	
3-methyl-2-thiabutane, $\text{CH}_3\text{SCH}(\text{CH}_3)_2$	c, l	1955	13-344		$62.88 \pm 0.12 (\ell) [77]$	
2-thiapentane, $\text{CH}_3\text{SC}_3\text{H}_7$	c, l	1957	13-326		$65.14 (\ell)$	[86]
3-thiapentane, $(\text{C}_2\text{H}_5)_2\text{S}$	c, l	1952	16-316		$64.36 \pm 0.10 (\ell) [89]$	
2,3-dithiabutane, $(\text{CH}_3\text{S})_2$	c, l	1950	13-352		$56.26 \pm 0.10 (\ell) [100]$ $80.54 \pm 0.30 (g) [100]$	
3,4-dithiahexane, $(\text{C}_2\text{H}_5\text{S})_2$	c, l	1952	13-299		$72.90 \pm 0.15 (\ell) [95]$	
4,5-dithiaoctane, $(\text{C}_3\text{H}_7\text{S})_2$	c, l	1958	12-351		$89.28 (\ell)$	[102]

## SECTION II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity °K	5 Relative Enthalpy Range °K	6 Entropy cal/deg-mole	7 Ref.
thiophene, $C_4H_4S$	c, l	1934 1949	238-289 12-336		$42.2 \pm 1.0$ (l) [103] $43.30 \pm 0.10$ (l) [101]	
2-methylthiophene, $(CH_3)_2C_4H_3S$	c, l	1956	12-344		52.22 (l)	[ 80 ]
3-methylthiophene, $(CH_3)_3C_4H_3S$	c, l	1953	12-337		52.185 $\pm 0.10$ (l) [ 83 ]	
benzothiophene, $C_8H_6S$	c, l	1954	12-330		42.329 $\pm 0.12$ (l)	[ 82 ]
thiacyclobutane, $(CH_2)_3S$	c, l	1953	12-321		$44.72 \pm 0.10$ (l) [ 93 ] $68.17 \pm 0.25$ (g) [ 93 ]	
thiacyclopentane, $(CH_2)_4S$	c, l	1952	13-333		49.67 $\pm 0.10$ (l)	[ 94 ]
thiacyclohexane, $(CH_2)_5S$	c, l	1954	13-342		52.16 $\pm 0.10$ (l)	[ 91 ]
<b>15. Amino acids, aliphatic groups</b>						
glycine, aminoacetic acid, $NH_2CH_2COOH$	c c	1933 1960	93-300 12-302		26.1 (c) 24.74 (c)	[ 61 ] [ 46 ]
d-alanine, l-2-amino propanoic acid, $CH_3(NH_2)CHCOOH$	c	1932	84-297		31.6 (c)	[ 55 ]
l-alanine, d-2-amino propanoic acid, $CH_3(NH_2)CHCOOH$	c	1960	12-305		30.88 (c)	[ 46 ]
dl-alanine, dl-2-amino propanoic acid, $CH_3(NH_2)CHCOOH$	c	1937	85-298		31.6 (c)	[ 53 ]

## SECTION II (Cont.)

1 Substances	2 Physical State	3 Year Reported	4 Heat Capacity Range °K	5 Relative Enthalpy Range °K	6 Entropy 298.15°K cal/deg-mole	7 Ref.
<i>L</i> -valine, <i>d</i> - $\alpha$ -aminoisovaleric acid, $(\text{CH}_3)_2\text{CH}(\text{NH}_2)\text{CHCOOH}$	c	1963	11-301	42.75	(c)	[44]
<i>L</i> -leucine, <i>L</i> - $\alpha$ -aminoisocaproic acid, $(\text{CH}_3)_2\text{CHCH}_2(\text{NH}_2)\text{CHCOOH}$	c	1963	11-305	50.62	(c)	[44]
<i>D,L</i> -leucine, <i>D,L</i> - $\alpha$ -aminoisocaproic acid, $(\text{CH}_3)_2\text{CHCH}_2(\text{NH}_2)\text{CHCOOH}$	c	1937	86-297	49.5	(c)	[53]
<i>L</i> -isoleucine, <i>d</i> - $\alpha$ -amino- $\beta$ -methylvaleric acid, $(\text{CH}_3)(\text{C}_2\text{H}_5)\text{CH}(\text{NH}_2)\text{CHCOOH}$	c	1963	11-306	49.71	(c)	[44]
<b>16. Amino acids, hydroxyl containing, aliphatic and aromatic groups</b>						
<i>L</i> -tyrosine, <i>L</i> - $\alpha$ -amino-p-hydroxyhydrocinnamic acid, $\text{HOCH}_6\text{CH}_4\text{CH}_2(\text{NH}_2)\text{CHCOOH}$	c	1937	87-295	53.0	(c)	[53]
	c	1963	11-302	51.15	(c)	[43]
<i>L</i> -serine, <i>L</i> - $\alpha$ -amino- $\beta$ -hydroxypropanoic acid, $\text{HOCH}_2(\text{NH}_2)\text{CHCOOH}$ , unpublished measurements: 10-305°K						
<i>L</i> -threonine, <i>L</i> - $\alpha$ -amino- $\beta$ -hydroxybutanoic acid, $\text{CH}_3\text{CHOH}(\text{NH}_2)\text{CHCOOH}$ , unpublished measurements: 10-305°K						
<b>17. Amino acids, aromatic and related groups</b>						
<i>L</i> -phenylalanine, <i>L</i> - $\alpha$ -amino- $\beta$ -phenylpropanoic acid, $\text{C}_6\text{H}_5\text{CH}_2(\text{NH}_2)\text{CHCOOH}$	c	1963	11-305	51.06	(c)	[43]
<i>L</i> -tryptophane, <i>L</i> - $\alpha$ -amino-3-indolepropanoic acid, $\text{C}_8\text{H}_6\text{NCH}_2(\text{NH}_2)\text{CHCOOH}$	c	1963	12-301	60.00	(c)	[43]

## SECTION II (Cont.)

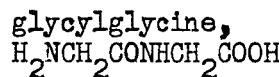
1	2	3	4	5	6	7
Substance	Physical State	Year Reported	Heat Capacity Range °K	Relative Enthalpy Enthalpy Range °K	298.15°K cal/deg-mole	Ref.
<b>18. Amino acids, carboxyl and amide groups</b>						
<i>l</i> -aspartic acid, <i>d</i> -aminosuccinic acid, $\text{HOOCCH}_2(\text{NH}_2)\text{CHCOOH}$	c c	1932 1963	88-294 11-301	41.5 (c) 40.66 (c)	[55] [45]	
<i>l</i> -asparagine, <i>l</i> - $\alpha$ -aminosuccinamic acid, $\text{NH}_2\text{COCH}_2(\text{NH}_2)\text{CHCOOH}$	c	1932	85-297	41.7 (c)	[55]	
<i>l</i> -asparagine monohydrate, <i>l</i> - $\alpha$ -aminosuccinamic acid monohydrate, $\text{NH}_2\text{COCH}_2(\text{NH}_2)\text{CHCOOH}$	c c	1932 1963	90-297 11-303	51.0 (c) 50.10 (c)	[55] [45]	
<i>d</i> -glutamic acid, <i>l</i> - $\alpha$ -aminoglutaric acid, $\text{HOOC}(\text{CH}_2)_2(\text{NH}_2)\text{CHCOOH}$	c	1932	91-295	45.7 (c)	[55]	
<i>d</i> -glutamic acid hydrochloride, <i>l</i> - $\alpha$ -aminoglutaric acid hydrochloride $\text{HOOC}(\text{CH}_2)_2(\text{NH}_3^+\text{Cl}^-)\text{CHCOOH}$	c	1940	85-297	59.33 (c)	[52]	
<i>l</i> -glutamic acid, <i>d</i> - $\alpha$ -aminoglutaric acid, $\text{HOOC}(\text{CH}_2)_2(\text{NH}_2)\text{CHCOOH}$	c	1963	9-303	44.98 (c)	[45]	
<i>l</i> -glutamine, <i>d</i> - $\alpha$ -aminoglutaramic acid, $\text{NH}_2\text{CO}(\text{CH}_2)_2(\text{NH}_2)\text{CHCOOH}$	c	1963	11-308	46.62 (c)	[45]	
<b>19. Amino acids, amino groups</b>						
<i>l</i> -lysine hydrochloride, <i>d</i> - $\alpha,\epsilon$ -diaminocaproic acid hydrochloride, $(\text{NH}_3^+\text{Cl}^-)(\text{CH}_2)_4(\text{NH}_2)\text{CHCOOH}$	c	1963	11-305	63.21 (c)	[42]	
<i>d</i> -arginine, <i>l</i> - $\alpha$ -amino- $\delta$ -guanidovaleric acid, $\text{NH}_2\text{C}(=\text{NH})\text{NH}(\text{CH}_2)_3(\text{NH}_2)\text{CHCOOH}$	c	1937	86-297	59.9 (c)	[53]	

## SECTION II (Cont.)

	1	2	3	4	5	6	7
Substance	Physical State	Year Reported	Heat Capacity Range °K	Relative Enthalpy Range °K	Enthalpy 298.15°K	Entropy cal/deg-mole	Ref.
<i>l</i> -arginine hydrochloride, <i>d</i> - $\alpha$ -amino- $\delta$ -guanidovaleric acid hydrochloride, $\text{NH}_2\text{C}(\text{=NH}_2\text{Cl})\text{ NH}(\text{CH}_2)_3(\text{NH}_2)\text{CHCOOH}$	c	1963	11-304		68.43 (c)	[42]	
<i>l</i> -histidine hydrochloride, <i>l</i> - $\alpha$ -amino-5-imidazole-propanoic acid hydrochloride, $\text{C}_3\text{H}_5\text{N}(\text{HCl})\text{ CH}_2(\text{NH}_2)\text{CHCOOH}$	c	1963	11-305		65.99 (c)	[42]	
<i>dl</i> -ornithine, <i>dl</i> - $\alpha$ - $\delta$ -diaminovaleric acid, $\text{NH}_2(\text{CH}_2)_3(\text{NH}_2)\text{CHCOOH}$	c	1940	89-298		46.2 (c)	[51]	
ornithine dihydrochloride, $\alpha$ - $\delta$ -diaminovaleric acid dihydrochloride, $(\text{NH}_3\text{Cl})(\text{CH}_2)_3(\text{NH}_3\text{Cl})\text{CHCOOH}$	c	1940	85-293		70.25 (c)	[52]	
<i>dl</i> -citrulline, <i>dl</i> - $\alpha$ -amino- $\delta$ -ureidovaleric acid, $\text{NH}_2\text{CONH}(\text{CH}_2)_3(\text{NH}_2)\text{CHCOOH}$	c	1940	89-301		60.8 (c)	[51]	
<b>20. Amino acids, sulfur containing groups</b>							
<i>l</i> -cysteine, <i>l</i> -2-amino-3-mercaptopropanoic acid, $\text{HSCH}_2(\text{NH}_2)\text{CHCOOH}$	c	1936	85-298		40.6 (c)	[7]	
<i>l</i> -cystine, <i>l</i> -3,3'-dithiobis(2-aminopropanoic acid), $(\text{HOOC}(\text{NH}_2)\text{CHCH}_2\text{S}-)_2$	c	1936	86-297		68.5 (c)	[7]	
	c	1964	11-303		67.06 (c)	[41]	
<i>l</i> -methionine, <i>l</i> -2-amino-4-methylthio-butanoic acid, $\text{CH}_3\text{S}(\text{CH}_2)_2(\text{NH}_2)\text{CHCOOH}$	c	1964	11-348		55.32 (c)	[41]	
<b>21. Amino acids, imino acid groups</b>							
<i>l</i> -proline, <i>l</i> -2-pyrrolidinecarboxylic acid, $\text{C}_4\text{H}_8\text{NCOOH}$	c	1940	88-300		40.8 (c)	[51]	
	c	1963	11-302		39.21 (c)	[43]	
<i>l</i> -hydroxyproline, <i>l</i> -4-hydroxy-2-pyrrolidine carboxylic acid, $\text{HO}(\text{C}_4\text{H}_7\text{N})\text{COOH}$ , unpublished measurements: 10-305°K							

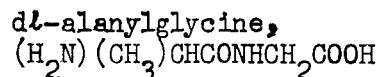
## SECTION II (Cont.)

1	2	3	4	5	6	7
Substance	Physical State	Year Reported	Heat Capacity Range °K	Relative Enthalpy Range °K	Entropy 298.15°K cal/deg-mole	Ref.

22. Other biologically important compounds, peptide bond

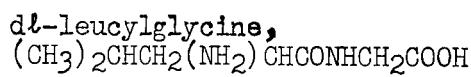
c 1941 87-294  
 unpublished measurements: 10-305°K

45.4 (c) [50]



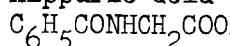
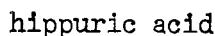
c 1941 85-296

51.0 (c) [50]



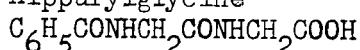
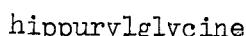
c 1941 86-297

67.2 (c) [50]



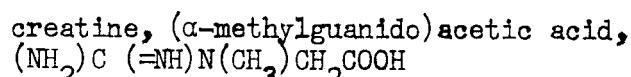
c 1941 85-298

57.2 (c) [50]



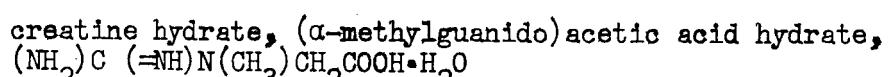
c 1941 85-297

75.2 (c) [50]

23. Other biologically important compounds, guanido group

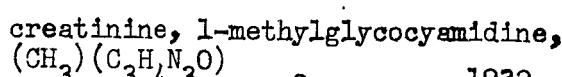
c 1932 87-296

45.3 (c) [55]



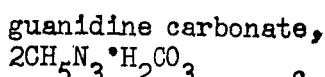
c 1940 87-298

56.0 (c) [51]



c 1932 87-296

40.0 (c) [55]



c 1940 86-298

70.59 (c) [52]

## SECTION II (Cont.)

1	2	3	4	5	6	7
Substance	Physical State	Year Reported	Heat Capacity Range °K	Relative Enthalpy Range °K	Entropy 298.15°K cal/deg-mole	Ref.
<b>24. Other biologically important compounds, purines and others</b>						
hypoxanthine, 6-oxypurine, $C_5H_4N_4O$	c	1935	85-298		34.8 (c)	[54]
xanthine, 2,6-dioxypurine, $C_5H_4N_4O_2$	c	1935	85-298		38.5 (c)	[54]
uric acid, 2,6,8-trioxypurine, $C_5H_4N_4O_3$	c	1935	86-297		41.4 (c)	[54]
adenine, 6-aminopurine, $C_5H_3N_4(NH_2)_2$	c	1935	88-298		36.1 (c)	[54]
guanine, 2-amino-6-hydroxypurine, $(H_2N)C_5H_2N_4(OH)_2$	c	1935	84-297		38.3 (c)	[54]
allantoin, 5-ureidohydantoin, $NH_2CONH(C_3H_3N_2O_2)_2$	c	1935	85-297		46.6 (c)	[54]
alloxan, pyrimidinetetrone, $C_4H_2N_2O_4$	c	1935	86-297		44.6 (c)	[54]
taurine, 2-aminoethanesulfonic acid, $(NH_2)_2(CH_2)_2SO_3^H$	c	1940	87-300		36.8 (c)	[51]

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### Section III

#### Preliminary Compilation and Illustrative Format of Data on Heats and Free Energies of Reaction and Formation

##### Bibliography on Amino Acids

George T. Armstrong and M. C. Bracken

1. C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub> (c) BIO-10

Alpha aminoacetic acid Glycine

CH<sub>2</sub>(NH<sub>2</sub>)COOH Amino Acid

Huffman, H. M., and Ellis, E. L., J. Am. Chem. Soc. 59, 2150-55 (1937). Thermal Data. VIII. The Heat Capacities, Entropies and Free Energies of Some Amino Acids.

2. C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub> (c) BIO-9

Alpha aminoacetic acid Glycine

CH<sub>2</sub>(NH<sub>2</sub>)COOH Amino Acid

Huffman, H. M., Fox, S. W., and Ellis, E. L., J. Am. Chem. Soc. 59, 2144-50 (1937).

Thermal Data. VII. The Heats of Combustion of Seven Amino Acids.

3. C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub> (c) BIO-2

Alpha aminoacetic acid Glycine

CH<sub>2</sub>(NH<sub>2</sub>)COOH Amino Acid

Stohmann, F., and Langbein, H., J. Prakt. Chem. 44, 336-99 (1891). Calorimetrische Untersuchungen. Ueber den Warmewerth der Nahrungsbestandtheile und deren Derivate.

4. C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub> (c) BIO-1

Alpha aminoacetic acid Glycine

CH<sub>2</sub>(NH<sub>2</sub>)COOH Amino Acid

Wrede, F., Z. Phys. Chem. 75, 81-94 (1910).  
Über die Bestimmung von Verbrennungswärmern mittels der kalorimetrischen Bombe unter Benutzung des Platinwiderstandsthermometers.

5. C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>(c) BIO-4

Alpha aminopropionic acid Alanine

CH<sub>3</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H Amino Acid

Berthelot, M. P., and Andre, G., Ann. Chim. Phys. [6] 27, 5-17 (1891).  
Sur Les Chaleurs De Formation Et De Combustion De Divers Principes Azotes,  
Derives Des Matieres Albuminoïdes.

6. C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>(c) BIO-3

Alpha amino propionic acid Alanine

CH<sub>3</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H Amino Acid

Fischer, E., and Wrede, F., Sitzber. Deut. Akad. Wiss. Berlin, Kl. Math.,  
Phys., Tech. 1904, 687-715.  
Über die Verbrennungswärme einiger organischer Verbindungen.

7. C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>(c) BIO-6

Alpha aminopropionic acid Alanine

CH<sub>3</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H Amino Acid

Landrieu, Ph., Compt. Rend. 142, 580-4 (1906).  
Thermochimie des hydrazones et des osazones, des dicetones- $\alpha$  et des sucre  
reducteurs.

8. C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>(c) BIO-1

Alpha aminopropionic acid d-Alanine

CH<sub>3</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H Amino Acid

Wrede, F., Z. Phys. Chem. 75, 81-94 (1910).  
Über die Bestimmung von Verbrennungswärmern mittels der kalorimetrischen  
Bombe unter Benutzung des Platinwiderstandsthermometers.

9. C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>(c) BIO-12  
Alpha aminopropionic acid                    l-Alanine  
CH<sub>3</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H                    Amino Acid  
  
Burton, K., and Krebs, H. A., Biochem. J. 54, 94-107 (1953).  
The Free-energy Changes Associated with the Individual Steps of the Tri-carboxylic Acid Cycle, Glycolysis and Alcoholic Fermentation and with the Hydrolysis of the Pyrophosphate Group of Adenosinetriphosphate.
10. C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>(c) BIO-12  
Alpha-aminopropionic acid                    dl-Alanine  
CH<sub>3</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H                    Amino Acid  
  
Burton, K., and Krebs, H. A., Biochem. J. 54, 94-107 (1953).  
The Free-energy Changes Associated with the Individual Steps of the Tri-carboxylic Acid Cycle, Glycolysis and Alcoholic Fermentation and with the Hydrolysis of the Pyrophosphate Group of Adenosinetriphosphate.
11. C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>(c) BIO-10  
Alpha-aminopropionic acid                    dl-Alanine  
CH<sub>3</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H                    Amino Acid  
  
Huffman, H. M., and Ellis, E. L., J. Am. Chem. Soc. 59, 2150-55 (1937).  
Thermal Data. VIII. The Heat Capacities, Entropies and Free Energies of Some Amino Acids.
12. C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>(c) BIO-9  
Alpha-aminopropionic acid                    dl-Alanine  
CH<sub>3</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H                    Amino Acid  
  
Huffman, H. M., Fox, S. W., and Ellis, E. L., J. Am. Chem. Soc. 59, 2144-50 (1937).  
Thermal Data. VII. The Heats of Combustion of Seven Amino Acids.

13. C<sub>3</sub>H<sub>7</sub>N<sub>0</sub>2 (c)

BIO-1

Alpha-aminopropionic acid                    dl-Alanine

CH<sub>3</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H                    Amino Acid

Wrede, F., Z. Phys. Chem. 75, 81-94 (1910).

Über die Bestimmung von Verbrennungswärmern mittels der kalorimetrischen Bombe unter Benutzung des Platinwiderstandsthermometers.

14. C<sub>3</sub>H<sub>7</sub>N<sub>0</sub>2 (c)

BIO-5

N-methylaminoacetic acid                    Sarcosine

CH<sub>3</sub>NHCH<sub>2</sub>COOH                    Amino Acid

Stohmann, F., and Langbein, H., J. Prakt. Chem. [2] 45, 305-56 (1892).  
Calorimetrische Untersuchungen. Ueber den Warmewerth von Kohlehydraten,  
mehrsaurigen Alkoholen und Phenolen.

15. C<sub>3</sub>H<sub>7</sub>N<sub>0</sub>2S (c)

BIO-11

Alpha-amino beta-mercaptopropionic acid Cysteine

HSCH<sub>2</sub>CH(NH<sub>2</sub>)COOH                    Amino Acid

Kolthoff, I. M., Stricks, W., and Tanaka, N., J. Am. Chem. Soc. 77, 4739-42  
(1955).

The Polarographic Prewaves of Cystine (RSSR) and Dithiodiglycolic Acid (TSST)  
and the Oxidation Potentials of the Systems RSSR-RSH and TSST-TSH.

16. C<sub>3</sub>H<sub>7</sub>N<sub>0</sub>3 (c)

BIO-13

Alpha-amino beta-hydroxypropionic acid Serine

CH<sub>2</sub>(OH)CH(NH<sub>2</sub>)COOH                    Amino Acid

Metzler, D. E., Longenecker, J. B., and Snell, E. E., J. Am. Chem. Soc. 76,  
639-44 (1954).

The Reversible Catalytic Cleavage of Hydroxy-amino Acids by Pyridoxal and  
Metal Salts.

17. C<sub>3</sub>H<sub>7</sub>N<sub>0</sub>3 (c) BIO-3
- |  |            |
|--|------------|
| Alpha-hydroxy beta-aminopropionic acid     | Isoserine  |
| NH <sub>2</sub> CH <sub>2</sub> CH(OH)COOH | Amino Acid |
- Fischer, E., and Wrede, F., Sitzber. Deut. Akad. Wiss. Berlin, Kl. Math., Phys., Tech. 1904, 687-715.  
Uber die Verbrennungswärme einiger organischer Verbindungen.
18. C<sub>3</sub>H<sub>7</sub>N<sub>0</sub>3 (c) BIO-1
- |  |            |
|--|------------|
| Alpha-hydroxy beta-aminopropionic acid     | Isoserine  |
| NH <sub>2</sub> CH <sub>2</sub> CH(OH)COOH | Amino Acid |
- Wrede, F., Z. Phys. Chem. 75, 81-94 (1910).  
Uber die Bestimmung von Verbrennungswärmen mittels der kalorimetrischen Bombe unter Benutzung des Platinwiderstandsthermometers.
19. C<sub>4</sub>H<sub>7</sub>N<sub>0</sub>4 (c) BIO-8
- |                                       |                     |
|---------------------------------------|---------------------|
| Iminodiacetic acid                    | Diglycolamidic acid |
| NH(CH <sub>2</sub> COOH) <sub>2</sub> | Amino Acid          |
- Stohmann, F., and Langbein, H., J. Prakt. Chem. [2], 49, 483-500 (1894).  
Calorimetrische Untersuchungen. Ueber die Thermischen Vorgänge bei der Bildung einiger Aminosäuren und Nitrile.
20. C<sub>4</sub>H<sub>7</sub>N<sub>0</sub>4 (c) BIO-4
- |  |               |
|--|---------------|
| Alpha-aminosuccinic acid                     | Aspartic acid |
| HOOCCH <sub>2</sub> CH(NH <sub>2</sub> )COOH | Amino Acid    |
- Berthelot, M. P., and Andre, G., Ann. Chim. Phys. [6] 27, 5-17 (1891).  
Sur Les Chaleurs De Formation Et De Combustion De Divers Principes Azotes, Derives Des Matieres Albuminoïdes.

21. C<sub>4</sub>H<sub>7</sub>N<sub>0</sub>4 (c) BIO-3

Alpha-aminosuccinic acid Aspartic acid

HOOCCH<sub>2</sub>CH(NH<sub>2</sub>)COOH Amino Acid

Fischer, E., and Wrede, F., Sitzber. Deut. Akad. Wiss. Berlin, Kl. Math., Phys., Tech. 1904, 687-715.  
Uber die Verbrennungswarme einiger organischer Verbindungen.

22. C<sub>4</sub>H<sub>7</sub>N<sub>0</sub>4 (c) BIO-7

Alpha-aminosuccinic acid Aspartic Acid

HOOCCH<sub>2</sub>CH(NH<sub>2</sub>)COOH Amino Acid

Stohmann, F., Z. Phys. Chem. 10, 410-24 (1892).  
Die Verbrennungswarmen organischer Verbindungen.

23. C<sub>4</sub>H<sub>7</sub>N<sub>0</sub>4 (c) BIO-12

Alpha-aminosuccinic acid L-Aspartic Acid

HOOCCH<sub>2</sub>CH(NH<sub>2</sub>)COOH Amino Acid

Burton, K., and Krebs, H. A., Biochem. J. 54, 94-107 (1953).  
The Free-energy Changes Associated with the Individual Steps of the Tri-carboxylic Acid Cycle, Glycolysis and Alcoholic Fermentation and with the Hydrolysis of the Pyrophosphate Group of Adenosinetriphosphate.

24. C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub> (c) BIO-2

Alpha-aminosuccinic acid monamide Asparagine

CH(NH<sub>2</sub>)CO<sub>2</sub>HCH<sub>2</sub>CONH<sub>2</sub> Amino Acid

Stohmann, F., and Langbein, H., J. Prakt. Chem. 44, 336-99 (1891).  
Calorimetrische Untersuchungen. Ueber den Warmewerth der Nahrungs-bestandtheile und deren Derivate.

25. C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub> (c)

BIO-3

Glycylglycine



Amino Acid

Fischer, E., and Wrede, F., Sitzber. Deut. Akad. Wiss. Berlin, Kl. Math., Phys., Tech. 1904, 687-715.

Über die Verbrennungswärme einiger organischer Verbindungen.

26. C<sub>4</sub>H<sub>9</sub>N<sub>0</sub>3 (c)

BIO-13

Alpha-amino beta-hydroxybutyric acid

l-Threonine



Amino Acid

Metzler, D. E., Longenecker, J. B., and Snell, E. E., J. Am. Chem. Soc. 76, 639-44 (1954).

The Reversible Catalytic Cleavage of Hydroxy-amino Acids by Pyridoxal and Metal Salts.

27. C<sub>5</sub>H<sub>8</sub>N<sub>2</sub>O<sub>5</sub> (c)

BIO-3

Glycylglycinecarboxylic acid



Amino Acid

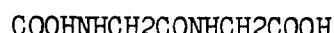
Fischer, E., and Wrede, F., Sitzber. Deut. Akad. Wiss. Berlin, Kl. Math., Phys., Tech. 1904, 687-715.

Über die Verbrennungswärme einiger organischer Verbindungen.

28. C<sub>5</sub>H<sub>8</sub>N<sub>2</sub>O<sub>5</sub> (c)

BIO-1

Glycylglycinecarboxylic acid



Amino Acid

Wrede, F., Z. Phys. Chem. 75, 81-94 (1910).

Über die Bestimmung von Verbrennungswärmern mittels der kalorimetrischen Bombe unter Benutzung des Platinwiderstandsthermometers.

29. C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub> (c) BIO-3
- |  |               |
|--|---------------|
| Alpha-aminoglutaric acid                                     | Glutamic Acid |
| HOOC(CH <sub>2</sub> ) <sub>2</sub> CH(NH <sub>2</sub> )COOH | Amino Acid    |
- Fischer, E., and Wrede, F., Sitzber. Deut. Akad. Wiss. Berlin, Kl. Math., Phys., Tech. 1904, 687-715.  
Über die Verbrennungswärme einiger organischer Verbindungen.
30. C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub> (c) BIO-12
- |  |                 |
|--|-----------------|
| Alpha-aminoglutaric acid                                     | L-Glutamic Acid |
| HOOC(CH <sub>2</sub> ) <sub>2</sub> CH(NH <sub>2</sub> )COOH | Amino Acid      |
- Burton, K., and Krebs, H. A., Biochem. J. 54, 94-107 (1953).  
The Free-energy Changes Associated with the Individual Steps of the Tricarboxylic Acid Cycle, Glycolysis and Alcoholic Fermentation and with the Hydrolysis of the Pyrophosphate Group of Adenosinetriphosphate.
31. C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub> (c) BIO-1
- |  |            |
|--|------------|
| Alpha-aminoisovaleric acid                                 | Valine     |
| (CH <sub>3</sub> ) <sub>2</sub> CHCH(NH <sub>2</sub> )COOH | Amino Acid |
- Wrede, F., Z. Phys. Chem. 75, 81-94 (1910).  
Über die Bestimmung von Verbrennungswärmern mittels der kalorimetrischen Bombe unter Benutzung des Platinwiderstandsthermometers.
32. C<sub>6</sub>H<sub>9</sub>NO<sub>6</sub> (c) BIO-8
- |                                      |                      |
|--------------------------------------|----------------------|
| N(CH <sub>2</sub> COOH) <sub>3</sub> | Triglycolamidic acid |
|                                      | Amino Acid           |
- Stohmann, F., and Langbein, H., J. Prakt. Chem. [2], 49, 483-500 (1894).  
Calorimetrische Untersuchungen. Ueber die Thermischen Vorgänge bei der Bildung einiger Aminsauren und Nitrile.

33. C<sub>6</sub>H<sub>11</sub>N<sub>3</sub>O<sub>4</sub> (c)

BIO-1

Diglycylglycine

Amino Acid

Wrede, F., Z. Phys. Chem. 75, 81-94 (1910).

Über die Bestimmung von Verbrennungswärmen mittels der kalorimetrischen Bombe unter Benutzung des Platinwiderstandsthermometers.

34. C<sub>6</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub> (c)

BIO-11

Di-(alpha-amino-beta thiopropionic) acid      Cystine

[ -SCH<sub>2</sub>CH(NH<sub>2</sub>)COOH]<sub>2</sub>      Amino Acid

Kolthoff, I. M., Stricks, W., and Tanaka, N., J. Am. Chem. Soc. 77, 4739-42 (1955).

The Polarographic Prewaves of Cystine (RSSR) and Dithiodiglycolic Acid (TSST) and the Oxidation Potentials of the Systems RSSR-RSH and TSST-TSH.

35. C<sub>6</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub> (c)

BIO-4

Alpha-aminoisocaproic acid      Leucine

(CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH(NH<sub>2</sub>)COOH      Amino Acid

Berthelot, M. P., and Andrie, G., Ann. Chim. Phys. [6] 27, 5-17 (1891).  
Sur Les Chaleurs De Formation Et De Combustion De Divers Principes Azotes,  
Derives Des Matieres Albuminoides.

36. C<sub>6</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub> (c)

BIO-3

Alpha-aminoisocaproic acid      Leucine

(CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH(NH<sub>2</sub>)COOH      Amino Acid

Fischer, E., and Wrede, F., Sitzber. Deut. Akad. Wiss. Berlin, Kl. Math.,  
Phys., Tech. 1904, 687-715.  
Über die Verbrennungswärme einiger organischer Verbindungen.

37. C<sub>6</sub>H<sub>13</sub>N<sub>0</sub><sub>2</sub> (c)

BIO-2

### Alpha-aminoisocaproic acid

### Leucine

$$(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{NH}_2)\text{COOH}$$

### Amino Acid

Stohmann, F., and Langbein, H., J. Prakt. Chem. 44, 336-99 (1891).  
Calorimetrische Untersuchungen. Ueber den Warmewerth der Nahrungs-  
bestandtheile und deren Derivate.

38. C<sub>6</sub>H<sub>13</sub>N<sub>0</sub><sub>2</sub> (c)

BIO-10

## Alpha-aminoisocaproic acid

### d-Leucine

$$(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{NH}_2)\text{COOH}$$

### Amino Acid

Huffman, H. M., and Ellis, E. L., J. Am. Chem. Soc. 59, 2150-55 (1937).  
Thermal Data. VIII. The Heat Capacities, Entropies and Free Energies of  
Some Amino Acids.

39. C<sub>6</sub>H<sub>13</sub>N<sub>0</sub>2 (c)

B10-9

### Alpha-aminoisocaproic acid

### d-Leucine

$$(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{NH}_2)\text{COOH}$$

### Amino Acid

Huffman, H. M., Fox, S. W., and Ellis, E. L., J. Am. Chem. Soc. 59, 2144-50 (1937).

## Thermal Data. VII. The Heats of Combustion of Seven Amino Acids.

40. C<sub>6</sub>H<sub>13</sub>N<sub>0</sub><sub>2</sub> (c)

BIO-10

### Alpha-aminoisocaproic acid

### l-Leucine

$$(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{NH}_2)\text{COOH}$$

### Amino Acid

Huffman, H. M., and Ellis, E. L., J. Am. Chem. Soc. 59, 2150-55 (1937).  
 Thermal Data. VIII. The Heat Capacities, Entropies and Free Energies of Some Amino Acids.

41. C<sub>6</sub>H<sub>13</sub>N<sub>0</sub><sub>2</sub> (c) BIO-9
- |  |            |
|--|------------|
| Alpha-aminoisocaproic acid   | l-Leucine  |
| (CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> CH(NH <sub>2</sub> )COOH | Amino Acid |
- Huffman, H. M., Fox, S. W., and Ellis, E. L., J. Am. Chem. Soc. 59, 2144-50 (1937).  
 Thermal Data. VII. The Heats of Combustion of Seven Amino Acids.
42. C<sub>6</sub>H<sub>13</sub>N<sub>0</sub><sub>2</sub> (c) BIO-10
- |  |            |
|--|------------|
| Alpha-aminoisocaproic acid   | dl-Leucine |
| (CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> CH(NH <sub>2</sub> )COOH | Amino Acid |
- Huffman, H. M., and Ellis, E. L., J. Am. Chem. Soc. 59, 2150-55 (1937).  
 Thermal Data. VIII. The Heat Capacities, Entropies and Free Energies of Some Amino Acids.
43. C<sub>6</sub>H<sub>13</sub>N<sub>0</sub><sub>2</sub> (c) BIO-9
- |  |            |
|--|------------|
| Alpha-aminoisocaproic acid   | dl-Leucine |
| (CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> CH(NH <sub>2</sub> )COOH | Amino Acid |
- Huffman, H. M., Fox, S. W., and Ellis, E. L., J. Am. Chem. Soc. 59, 2144-50 (1937).  
 Thermal Data. VII. The Heats of Combustion of Seven Amino Acids.
44. C<sub>6</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub> (c) BIO-9
- |  |            |
|--|------------|
| Alpha-amino-delta-guanidovaleric acid  | Arginine   |
| H <sub>2</sub> NC(=NH)NHCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(NH <sub>2</sub> )COOH | Amino Acid |
- Huffman, H. M., Fox, S. W., and Ellis, E. L., J. Am. Chem. Soc. 59, 2144-50 (1937).  
 Thermal Data. VII. The Heats of Combustion of Seven Amino Acids.

45. C<sub>6</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub> (c) BIO-10  
Alpha amino-delta-guanidovaleric acid d-Arginine  
H2NC(=NH)NHCH2CH2CH2CH(NH2)COOH Amino Acid  
Huffman, H. M., and Ellis, E. L., J. Am. Chem. Soc. 59, 2150-55 (1937).  
Thermal Data. VIII. The Heat Capacities, Entropies and Free Energies of  
Some Amino Acids.
46. C<sub>7</sub>H<sub>13</sub>N<sub>0</sub><sub>3</sub> (c) BIO-1  
Formyl-d, l-leucine  
Amino Acid  
Wrede, F., Z. Phys. Chem. 75, 81-94 (1910).  
Über die Bestimmung von Verbrennungswärmern mittels der kalorimetrischen  
Bombe unter Benutzung des Platinwiderstandsthermometers.
47. C<sub>8</sub>H<sub>14</sub>N<sub>4</sub>O<sub>5</sub> (c) BIO-1  
Triglycylglycine  
Amino Acid  
Wrede, F., Z. Phys. Chem. 75, 81-94 (1910).  
Über die Bestimmung von Verbrennungswärmern mittels der kalorimetrischen  
Bombe unter Benutzung des Platinwiderstandsthermometers.
48. C<sub>8</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub> (c) BIO-1  
d-l-Leucylglycine  
Amino Acid  
Wrede, F., Z. Phys. Chem. 75, 81-94 (1910).  
Über die Bestimmung von Verbrennungswärmern mittels der kalorimetrischen  
Bombe unter Benutzung des Platinwiderstandsthermometers.



53. C<sub>10</sub>H<sub>19</sub>N<sub>3</sub>O<sub>4</sub> (c)

BIO-3

Leucylglycylglycine

(CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH(NH<sub>2</sub>)CONHCH<sub>2</sub>CONHCH<sub>2</sub>COOH

Amino Acid

Fischer, E., and Wrede, F., Sitzber. Deut. Akad. Wiss. Berlin, Kl. Math.,  
Phys., Tech. 1904, 687-715.  
Uber die Verbrennungswärme einiger organischer Verbindungen.

UNITED STATES GOVERNMENT

U.S. DEPARTMENT OF COMMERCE  
NATIONAL BUREAU OF STANDARDS

# Memorandum

TO : G. W. Beckett - NBS  
G. T. Furukawa  
J. Hilsenrath  
G. Jacobs - NASA  
F. H. Quimby  
H. Morowitz - Yale University

FROM : G. T. Armstrong *George T. Armstrong*

DATE: August 11, 1964

SUBJECT: Planning Session August 6, 1964  
CHNOPS Compounds  
NBS Project 221-11-0429; NASA Contract R-138

At our request, Dr. Harold Morowitz from the Yale University Department of Molecular Biology and Biophysics visited us and discussed plans for subject program on Exobiology. Also present were Dr. George Jacobs and Dr. Freeman Quimby, of NASA Exobiology branch, Dr. Takehiko Shimanouchi of the University of Tokyo, as well as NBS staff members, G. T. Armstrong, C. W. Beckett, G. T. Furukawa and J. Hilsenrath.

In a preliminary lecture Morowitz outlined the overall problem. Then Armstrong outlined the NBS organization to undertake the work, and progress in the month of July, represented by a report now in preparation. Furukawa described the progress of his review of heat capacity data, and Hilsenrath indicated machine computation problems and the approach to solving them. At the present point it appears that a scaling technique of some kind can be used to handle overflow in the computer, but this has not been fully tested.

Morowitz outlined a procedure for selecting compounds for examination of which he presented a preliminary list of about 100 (appended). His proposed categories include (a) zero carbon, (b) one carbon, (c) two carbon. Dr. Morowitz's categories will be used to form a starting list for study and will be amplified as other compounds in these categories are encountered. He suggested that a list comprised of compounds in these categories be all one should include in a preliminary testing of the equilibrium calculations. By examination of the low yield compounds, the number of applicable substances could be narrowed at each stage of added complexity of the products, and thus the way paved for extension to more complicated systems. An additional category (d) three carbon molecules probably provide the limit to which a systematic inclusion of all known compounds can be included.

MEMORANDUM (Cont.)

Planning Session  
CHNOPS Compounds

August 11, 1964

Beckett suggested inclusion of some active species such as free radicals which would not be present in large amounts at low temperature but would definitely be formed in energy-rich reaction zones. The known molecules of this type can be included in the foregoing categories (a-d) and will be included in the search for data.

Some discussion of more complex life-related compounds indicated that the chemistry of them would probably be most important in aqueous phases, and that proper treatment of them would not be easy at least in the initial stages of the study. However, Morowitz agreed to prepare and supply a list of "ubiquitous" compounds occurring in all living organisms which he estimated at about 200 in number selected from the 1300 compounds listed in "Pfizer Handbook of Microbial Metabolites" (McGraw Hill, 1961). This list will later be combined with lists of compounds containing "zero", one, two, and three carbon atoms and the other elements: HNOPS of greatest interest.

Dr. Morowitz will be retained as consultant for this project on a formal basis as soon as possible.

The meeting started at 10:00 A.M. and adjourned about 2:45 P.M.

## COMPOUNDS

CHN	Hydrocyanic Acid
CHNO	Cyanic Acid
CHNS	Thiocyanic Acid
CHN <sub>3</sub> O <sub>6</sub>	Nitroform
CH <sub>2</sub> N <sub>2</sub> <sup>3</sup> <sub>6</sub>	Cyanamide, Diazomethane
CH <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	Formonitriolic Acid
CH <sub>2</sub> N <sub>2</sub> O <sub>4</sub>	Dinitromethane
CH <sub>2</sub> N <sub>4</sub>	1, 2, 3, 4-Tetrazole
CH <sub>2</sub> O	Formaldehyde
(CH <sub>2</sub> O) <sub>x</sub>	Polyoxymethane
CH <sub>2</sub> O <sub>2</sub>	Formic Acid
CH <sub>2</sub> S <sub>3</sub>	Trithiocarbonic Acid
CH <sub>3</sub> NO	Formaldehyde Oxime, Formamide
CH <sub>3</sub> NO <sub>2</sub>	Nitromethane, Methyl Nitrite
CH <sub>3</sub> NO <sub>3</sub>	Methylnitrate
CH <sub>3</sub> NS <sub>2</sub>	Dithiocarbamic Acid
CH <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	Nitrourea
CH <sub>4</sub>	Methane
CH <sub>4</sub> N <sub>2</sub> O	Formamidoxime, Formohydrazide Urea
CH <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	Hydroxyurea
CH <sub>4</sub> N <sub>2</sub> S	Thiourea
CH <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	Nitro Guanidine
CH <sub>4</sub> O	Methanol
CH <sub>4</sub> O <sub>3</sub> S	Methanesulfonic Acid
CH <sub>4</sub> O <sub>4</sub> S	Methylsulfuric Acid
CH <sub>4</sub> O <sub>6</sub> S <sub>2</sub>	Methionic Acid
CH <sub>4</sub> S	Methanethiol
CH <sub>5</sub> N	Methylamine
CH <sub>5</sub> NO	Methyl-hydroxylamine, Methoxyamine
CH <sub>5</sub> N <sub>3</sub>	Guanidine
CH <sub>5</sub> N <sub>3</sub> O	Semicarbazide
CH <sub>5</sub> N <sub>3</sub> O <sub>4</sub>	Urea-nitrate
CH <sub>5</sub> N <sub>3</sub> S	Thiosemicarbazide

## Compounds (Cont.)

$\text{CH}_5\text{O}_3\text{P}$	Methanephosphonic Acid
$\text{CH}_5\text{P}$	Methyl Phosphine
$\text{CH}_6\text{N}_2$	Methyl Hydrazine
$\text{CH}_6\text{N}_4$	1-Amino Guanidine
$\text{CH}_6\text{N}_4\text{O}$	Carbohydrazide
$(\text{CN})_x$	Paracyanogen
$\text{CN}_4\text{O}_8$	Tetranitromethane
CO	Carbon Monoxide
COS	Carbonyl Sulfide
$\text{CO}_2$	Carbon Dioxide
$\text{CS}_2$	Carbon Disulfide
$\text{CH}_6\text{N}_2\text{O}_2$	Ammonium Carbamate
$\text{CH}_8\text{N}_2\text{O}_3$	Ammonium Carbonate
$\text{CH}_5\text{NO}_3$	Ammonium Bicarbonate
$\text{CH}_4\text{N}_2\text{O}_2$	Ammonium Cyanate
$\text{CH}_4\text{N}_2$	Ammonium Cyanide
$\text{CH}_5\text{NO}_2$	Ammonium Formate
$\text{H}_5\text{NO}$	Ammonium Hydroxide
$\text{H}_4\text{N}_2\text{O}_3$	Ammonium Nitrate
$\text{H}_4\text{N}_2\text{O}_2$	Ammonium Nitrite
$\text{H}_{10}\text{N}_2\text{O}_6\text{P}_2$	Ammonium Hydrophosphate
$\text{H}_9\text{N}_2\text{O}_4\text{P}$	Ammonium Orthophosphate Mono H
$\text{H}_6\text{NO}_4\text{P}$	Ammonium Orthophosphate di H
$\text{H}_6\text{NO}_2\text{P}$	Ammonium Hydrophosphite
$\text{H}_6\text{NO}_3\text{P}$	Ammonium Orthophosphite di H
$\text{H}_6\text{N}_2\text{O}_3\text{S}$	Ammonium Sulfamate
$\text{H}_8\text{N}_2\text{O}_4\text{S}$	Ammonium Sulfate
$\text{H}_5\text{NO}_4\text{S}$	Ammonium Bisulfate
$\text{H}_8\text{N}_2\text{O}_8\text{S}_2$	Ammonium Peroxidisulfate
$\text{H}_8\text{N}_2\text{S}$	Ammonium Sulfide Mono
$\text{H}_5\text{NS}$	Ammonium Sulfide Hydro
$\text{H}_{10}\text{N}_2\text{O}_4\text{S}$	Ammonium Sulfite

**Compounds (Cont.)**

$\text{H}_5\text{NO}_3\text{S}$	Ammonium Bisulfite
$\text{CH}_5\text{N}_2\text{S}$	Ammonium Thriocyanate
$\text{H}_{10}\text{N}_2\text{O}_7\text{S}_2$	Ammonium Dithionate
$\text{H}_8\text{N}_2\text{O}_3\text{S}_2$	Ammonium Thiosulfate
$\text{C}_3\text{O}_2$	Carbon Suboxide
$\text{C}_3\text{S}_2$	Carbon Subsulfide
$\text{CS}$	Carbon Monosulfide
$\text{H}_4\text{N}_2$	Hydrazine
$\text{H}_5\text{N}_5$	Hydrazine Azide
$\text{C}_2\text{H}_8\text{N}_2\text{O}_4$	Hydrazine Formate
$\text{H}_6\text{N}_2\text{O}$	Hydrazine Hydrate
$\text{H}_5\text{N}_3\text{O}_3$	Hydrazine Nitrate
$\text{H}_6\text{N}_4\text{O}_6$	Hydrazine Dinitrate
$\text{H}_8\text{N}_2\text{O}_6\text{P}_2$	Hydrazine Hypophosphate
$\text{H}_7\text{N}_2\text{O}_4\text{P}$	Hydrazine Orthophosphate
$\text{N}_2\text{H} \cdot \text{H}_3\text{PO}_4$	Hydrazine Mono-orthophosphite
$\text{N}_2\text{H} \cdot 2\text{H}_3\text{PO}_3$	Hydrazine Diorthophosphite
$\text{NH}_2\text{OH} \cdot \text{HNO}_3$	Hydroxylamine Nitrate
$2\text{NH}_2\text{OH} \cdot \text{H}_2\text{SO}_4$	Hydroxalamine Sulfate
$\text{H}$	Hydrogen
$\text{H}_2\text{O}$	Water
$\text{H}_2\text{O}_2$	Hydrogen Peroxide
$\text{H}_3\text{P}$	Hydrogen Phosphide A
$\text{H}_4\text{P}_2$	Hydrogen Phosphide B
$(\text{H}_2\text{P}_4)_3$	Hydrogen Phosphide C
$\text{H}_2\text{S}$	Hydrogen Sulfide
$\text{H}_2\text{S}_2$	Hydrogen Disulfide
$\text{H}_2\text{S}_3$	Hydrogen Trisulfide
$\text{H}_2\text{S}_5$	Hydrogen Pentasulfide
$\text{N}_2$	Nitrogen
$\text{N}_2\text{O}$	Nitrous Oxide

## Compounds (Cont.)

NO	Nitric Oxide
NO <sub>2</sub>	Nitrogen Dioxide
N <sub>2</sub> O <sub>3</sub>	Nitrogen Sesquionide
N <sub>2</sub> O <sub>5</sub>	Nitrogen Pentoxide
NO <sub>3</sub>	Nitrogen Trioxide
NOHSO <sub>4</sub>	Nitrosulfuric Acid
(NOSO <sub>3</sub> ) <sub>2</sub> O	Nitrosylsulfuric Acid
HNO <sub>3</sub>	Nitric Acid
HNO <sub>2</sub>	Nitrous Acid
H <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	Hyponitrous Acid
O <sub>2</sub>	Oxygen
(PH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	Phosphonium Sulfate